



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:27 AM GMT

PDB ID : 1A7R  
Title : FV FRAGMENT OF MOUSE MONOCLONAL ANTIBODY D1.3 (BALB/C, IGG1, K) VARIANT CHAIN L GLU81->ASP  
Authors : Marks, C.; Henrick, K.; Winter, G.  
Deposited on : 1998-03-16  
Resolution : 2.01 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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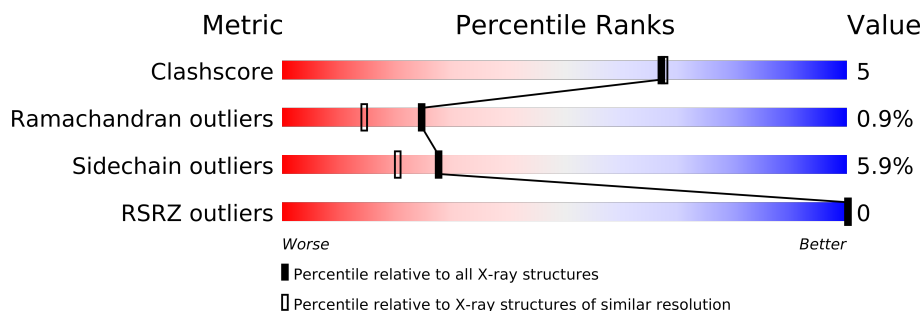
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	107	
2	H	116	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1832 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IGG1-KAPPA D1.3 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	107	Total	C	N	O	S	0	0	0
			816	518	135	161	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	VAL	GLU	CONFLICT	UNP P01635
L	50	TYR	LYS	CONFLICT	UNP P01635
L	51	THR	ALA	CONFLICT	UNP P01635
L	52	THR	GLN	CONFLICT	UNP P01635
L	81	ASP	GLU	VARIANT	UNP P01635
L	?	-	PRO	DELETION	UNP P01635
L	96	ARG	TRP	CONFLICT	UNP P01635

- Molecule 2 is a protein called IGG1-KAPPA D1.3 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	116	Total	C	N	O	S	0	1	0
			905	566	160	175	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	312	LEU	VAL	CONFLICT	UNP P01820

- Molecule 3 is water.

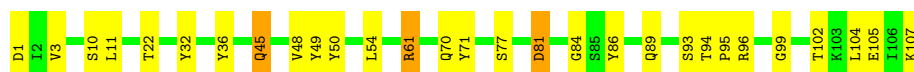
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	55	Total	O	0	0
			55	55		
3	L	56	Total	O	0	0
			56	56		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: IGG1-KAPPA D1.3 FV (LIGHT CHAIN)

Chain L: 



- Molecule 2: IGG1-KAPPA D1.3 FV (HEAVY CHAIN)

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.25Å 90.25Å 56.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.01 13.89 – 2.02	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.01) 97.1 (13.89-2.02)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.01Å)	Xtriage
Refinement program	CCP4	Depositor
R, $R_{free}$	0.170 , (Not available) 0.163 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 62.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 15330 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	L	1.28	2/837 (0.2%)	2.39	27/1138 (2.4%)
2	H	1.09	0/930	2.24	39/1261 (3.1%)
All	All	1.18	2/1767 (0.1%)	2.31	66/2399 (2.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	70	GLN	CB-CG	-16.71	1.07	1.52
1	L	61	ARG	NE-CZ	-5.00	1.26	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	61	ARG	CD-NE-CZ	39.47	178.86	123.60
2	H	266	ARG	NE-CZ-NH2	-19.64	110.48	120.30
1	L	96	ARG	NE-CZ-NH2	-15.55	112.53	120.30
2	H	266	ARG	NE-CZ-NH1	15.41	128.00	120.30
1	L	1	ASP	CB-CG-OD2	-15.18	104.64	118.30
1	L	105	GLU	OE1-CD-OE2	11.40	136.98	123.30
2	H	258	ASP	CB-CG-OD2	10.98	128.18	118.30
2	H	302	ARG	NE-CZ-NH2	-10.67	114.97	120.30
1	L	96	ARG	NH1-CZ-NH2	10.60	131.06	119.40
2	H	254	ASP	CB-CG-OD1	10.23	127.51	118.30
1	L	1	ASP	CB-CG-OD1	9.57	126.92	118.30
2	H	304	ASP	CB-CG-OD1	8.92	126.33	118.30
1	L	70	GLN	N-CA-CB	-8.54	95.22	110.60
2	H	301	TYR	CB-CG-CD1	-8.27	116.04	121.00
1	L	70	GLN	CA-CB-CG	8.07	131.15	113.40
2	H	258	ASP	CB-CG-OD1	-8.02	111.08	118.30
2	H	294	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	L	96	ARG	NE-CZ-NH1	-7.78	116.41	120.30
2	H	254	ASP	CB-CG-OD2	-7.72	111.35	118.30
2	H	228	SER	CB-CA-C	-7.50	95.85	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	218	LEU	CB-CG-CD1	7.45	123.66	111.00
2	H	294	TYR	CB-CG-CD1	7.43	125.45	121.00
1	L	86	TYR	CB-CG-CD2	-7.29	116.63	121.00
1	L	71	TYR	CB-CG-CD2	-7.18	116.69	121.00
2	H	206	GLU	OE1-CD-OE2	-7.04	114.85	123.30
1	L	10	SER	N-CA-CB	6.84	120.76	110.50
2	H	292	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	H	201	GLN	CA-C-O	6.69	134.15	120.10
1	L	49	TYR	CB-CG-CD1	-6.56	117.07	121.00
1	L	105	GLU	CG-CD-OE2	-6.37	105.56	118.30
2	H	228	SER	CA-CB-OG	-6.31	94.15	111.20
2	H	267	LEU	CB-CA-C	-6.26	98.30	110.20
2	H	289	ASP	CB-CG-OD2	6.26	123.93	118.30
2	H	259	TYR	CB-CG-CD1	-6.23	117.26	121.00
2	H	225	SER	N-CA-CB	6.21	119.82	110.50
2	H	284	SER	CA-C-N	-6.13	103.72	117.20
2	H	292	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	L	102	THR	N-CA-CB	6.00	121.69	110.30
1	L	81	ASP	CB-CG-OD1	5.99	123.69	118.30
1	L	49	TYR	CG-CD2-CE2	-5.84	116.63	121.30
2	H	213	ALA	N-CA-CB	-5.78	102.00	110.10
1	L	50	TYR	CG-CD2-CE2	-5.75	116.70	121.30
1	L	49	TYR	CB-CG-CD2	5.73	124.44	121.00
2	H	284	SER	CA-C-O	5.70	132.07	120.10
2	H	228	SER	N-CA-CB	5.65	118.97	110.50
2	H	297	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	H	218	LEU	CA-CB-CG	5.52	128.00	115.30
1	L	11	LEU	CA-CB-CG	5.50	127.95	115.30
2	H	246	GLU	OE1-CD-OE2	5.49	129.89	123.30
2	H	201	GLN	CA-C-N	-5.43	105.26	117.20
2	H	218	LEU	CB-CA-C	5.41	120.49	110.20
2	H	301	TYR	CB-CG-CD2	5.36	124.22	121.00
1	L	32	TYR	CG-CD2-CE2	-5.33	117.03	121.30
1	L	86	TYR	CB-CG-CD1	5.20	124.12	121.00
1	L	93	SER	N-CA-CB	-5.19	102.72	110.50
1	L	22	THR	O-C-N	5.18	130.99	122.70
1	L	45	GLN	CB-CG-CD	5.18	125.06	111.60
2	H	316	SER	N-CA-CB	-5.12	102.81	110.50
2	H	206	GLU	CG-CD-OE2	5.12	128.54	118.30
1	L	84	GLY	N-CA-C	-5.12	100.31	113.10
2	H	238	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	L	99	GLY	N-CA-C	-5.04	100.49	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	203	GLN	N-CA-CB	-5.03	101.55	110.60
2	H	201	GLN	CA-CB-CG	5.01	124.42	113.40
2	H	286	HIS	O-C-N	5.01	130.71	122.70
2	H	225	SER	CB-CA-C	-5.00	100.59	110.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	816	0	783	4	0
2	H	905	0	873	13	0
3	H	55	0	0	1	0
3	L	56	0	0	1	0
All	All	1832	0	1656	17	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (17) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:299[A]:ARG:NH1	2:H:302:ARG:NH2	2.24	0.85
2:H:218:LEU:HD12	2:H:282:MET:HB2	1.80	0.64
2:H:267:LEU:HD23	2:H:282:MET:HG2	1.88	0.56
1:L:3:VAL:HG12	3:L:424:HOH:O	2.08	0.53
2:H:299[A]:ARG:NH1	2:H:302:ARG:HH22	2.06	0.47
2:H:211:LEU:HD11	2:H:315:SER:CB	2.46	0.46
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.62	0.46
1:L:48:VAL:HG22	1:L:54:LEU:HD23	1.97	0.45
2:H:267:LEU:HD22	2:H:280:LEU:HD11	1.98	0.45
1:L:94:THR:HB	1:L:95:PRO:HA	1.99	0.44
2:H:201:GLN:N	2:H:201:GLN:OE1	2.51	0.43
2:H:222:CYS:HB2	2:H:236:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:299[A]:ARG:NH1	3:H:471:HOH:O	2.28	0.41
2:H:218:LEU:HB3	2:H:285:LEU:HD11	2.02	0.41
2:H:211:LEU:HD11	2:H:315:SER:HB2	2.02	0.41
2:H:209:PRO:CG	2:H:218:LEU:HD23	2.50	0.41
2:H:297:ARG:O	2:H:303:LEU:HA	2.20	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	22	12
2	H	115/116 (99%)	110 (96%)	4 (4%)	1 (1%)	25	14
All	All	220/223 (99%)	212 (96%)	6 (3%)	2 (1%)	25	14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	284	SER
1	L	77	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	89/91 (98%)	84 (94%)	5 (6%)	30	22
2	H	99/100 (99%)	93 (94%)	6 (6%)	26	19
All	All	188/191 (98%)	177 (94%)	11 (6%)	28	20

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	45	GLN
1	L	61	ARG
1	L	81	ASP
1	L	104	LEU
1	L	107	LYS
2	H	201	GLN
2	H	218	LEU
2	H	221	THR
2	H	261	SER
2	H	276	SER
2	H	315	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
2	H	201	GLN
2	H	256	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	L	107/107 (100%)	-0.56	0 100 100	9, 17, 29, 42	6 (5%)
2	H	116/116 (100%)	-0.47	0 100 100	7, 16, 30, 37	3 (2%)
All	All	223/223 (100%)	-0.51	0 100 100	7, 16, 29, 42	9 (4%)

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.